

On Lennard-Jones type potentials and hard-core potentials with an attractive tail

Thiago Morais^{1,3}, Aldo Procacci¹ and Benedetto Scoppola²

¹ Departamento de Matemática UFMG 30161-970 - Belo Horizonte - MG Brazil

² Dipartimento di Matematica Università “Tor Vergata” V.le ricerca scientifica 00100 - Roma - Italy

³ Departamento de Matemática UFOP 35400-000 - Ouro Preto - MG Brazil

July 2, 2014

Abstract

We revisit an old tree graph formula, namely the Brydges-Federbush tree identity, and use it to get new bounds for the convergence radius of the Mayer series for gases of continuous particles interacting via non absolutely summable pair potentials with an attractive tail including Lennard-Jones type pair potentials.

1 Introduction

The rigorous approach to the equilibrium statistical mechanics of rarefied gases of classical particles is among the most deeply studied subjects in area of mathematical physics. Most of the results in this research field have been obtained during the decade of the sixties. The rigorous analysis of the continuous gas of particles has been mainly developed by putting the system in the Grand Canonical Ensemble, in which there are three fixed thermodynamic parameters: the volume V (i.e. the system is confined in a large, typically cubic, box), the inverse temperature β and the fugacity λ . The total number of particles is not a fixed quantity. The logarithm of the normalization constant of the probability in such an ensemble (i.e. the so-called grand canonical partition function), divided by the volume, is proportional to the thermodynamic pressure of the system, while its derivative with respect to the fugacity λ is proportional to the density. Both pressure and density are functions of the two thermodynamic parameters β and λ . So, reexpressing the fugacity as a function of the density, one can get the pressure as a function of the temperature and density, i.e. the equation of state of the system. It is thus crucial to be able to calculate the logarithm of the grand canonical partition function in order to study the thermodynamic properties of these systems.

The logarithm of the partition function can be written formally in terms of a series in powers of the particle fugacity λ , known as the Mayer series, whose coefficients (the Mayer coefficients) depend on the volume V and on the inverse temperature β . Indeed, J. E. Mayer [17, 16] first gave the explicit expressions of the n -th order coefficient of this series in terms of a sum over connected graphs between n vertices of cluster integrals. An upper bound of the type $(\text{Const.})^n$ on these n -th order coefficients, where C is a constant (possibly depending on β), guarantees analyticity of the Mayer series, at least for sufficiently small activity values λ (depending on the temperature but uniform in the volume).

Such a kind of bound was generally considered very hard to obtain, due to the fact that the number C_n of connected graphs between n vertices is greater the order of C^{n^2} with $C > 1$ (indeed, by a simple counting argument it is easy to show that $C_n \geq 2^{(n-1)(n-2)/2}$). So the question regarding the convergence of this series (and the related virial series) remained unanswered until the beginning of the sixties.

The first breakthrough towards the rigorous analysis of the Mayer series for such systems was obtained in 1962 in a paper by Groeneveld [11], who gave, under the (severe) assumption that particles interact via a purely repulsive pair potential, a bound of the type $(\text{Const.})^n$ for the n -th order Mayer coefficient. Just one year later, Penrose [19, 20] and independently Ruelle [27, 28] proved that the Mayer series of a system of continuous particles is actually an analytic function for small values of the fugacity for a large class of pair interactions (the so-called stable and tempered pair potentials, see ahead for the definitions), as well as providing a lower bound for the convergence radius, which remains till nowadays the best available in the literature.

These impressive results were all obtained “indirectly”, i.e. not working directly on the explicit expressions of the Mayer coefficients in terms of sums over connected graphs by trying to bound them exploiting some cancelations. The indirect method used was based on the analysis of iterative relations between correlation functions of the system (the so-called Kirkwood-Salsburg Equations (KSE) [13]). A direct estimate on the Mayer coefficients was proposed some years later by Penrose [21] who however considered only systems of particles interacting via pair potentials in a quite restricted sub-class of the stable and tempered ones. Namely, pair potentials with a repulsive hard-core at short distance but possibly with a negative tail (i.e. attractive) at large distance. To get the “direct” bound, Penrose rewrote the sum over connected graphs of the n -th order Mayer coefficient in terms of trees, by grouping together some terms, obtaining, for the first time, a so-called *tree graph identity* (TGI). The method developed in [21] was simpler than the KSE technique used in [19, 20, 27, 28]. However, the lower bound on the convergence radius obtained by Penrose for such restricted class of pair potentials was identical to that obtained via KSE methods by Ruelle and himself in 1963. Probably for this reason this first example of TGI contained did not receive the attention it deserved. The potentiality of the Penrose TGI has been recently rescued in the recent works [6, 7, 8] where the Penrose TGI has been used to get improvements the cluster expansion convergence region of the abstract polymer gas [6], the zero-temperature antiferromagnetic Potts model on infinite graphs [7], and of the hard-sphere gas on the continuum[8].

An alternative TGI was proposed a decade later in a paper by Brydges and Federbush [4]. As far as absolutely summable potentials were considered, Brydges and Federbush were able to deduce new C^n bounds on the n order Mayer coefficient (and hence on the Mayer series convergence radius). These new bounds improved those obtained by Penrose and Ruelle for a significant subclass the of absolutely summable pair potentials. Nevertheless the requirement of absolute summability left out most of the physically relevant examples, such as the hard-sphere gas and the Lennard-Jones gas (both with non absolutely summable pair potentials due to their divergence at short distances). The Brydges-Federbush TGI had a much more successful career, especially in constructive field theory, and further developments of this identity were given by several authors (see e.g. [1], [5], [4], [25]). Anyway, the limitations on the pair potentials present both in the Penrose TGI and Brydges-Federbush TGI have substantially never been overcome and the old bound obtained by Penrose and Ruelle in 1963 via the KSE method remains until today the best available, valid moreover for the most general class of pair potentials, i.e. stable and tempered pair potentials.

A recent development of the Brydges-Federbush TGI was given by one of us in [23, 24], within the framework of the abstract polymer gas. This development allowed to derive a new tree graph

inequality (see formula (3.11) in [23], or Proposition 1 in [24]) which was used in [24] to construct a cluster expansion for abstract polymers interacting via a non purely hardcore pair potential. The results contained in [23, 24] strongly indicate that the range of application of the Brydges-Federbush TGI could be broadened even for continuous particle systems, beyond the class of absolutely summable pair potentials. Indeed, as pointed out by Poghosyan and Ueltschi in [22], the new inequality presented in [24, 23] can be used to get new bounds for the class of potentials considered by Penrose in 1967, e.g. short distance hard-core potentials with an attractive tail (Theorem 3 for Penrose potentials ahead), and these bounds were explicitly used in recent works by Jansen [12] and Tate [29].

In the present paper we analyze the Brydges-Federbush tree graph identity under the light of the developments of [23, 24]. We first revisit, for pedagogical purpose, the tree graph inequality obtained in [24, 23] and illustrate how from this inequality it is possible to obtain straightforwardly the new bounds for Penrose potentials given in [22] (formula (3.7), Theorem 4 below). We then present a new tree graph inequality (formula (3.12), Theorem 7 below) which yields alternative bounds for a wide class of non-absolutely summable pair potentials with significant importance in physics. This class includes the Lennard-Jones type potentials (see definition ahead) for which we are thus able to produce new bounds alternative to the classical Ruelle-Penrose bounds. We also conjecture that this class actually coincides with the whole class of stable and tempered potentials.

While it is easy to see that the inequality (3.7) provides a clearly improved bound with respect to the classical Penrose-Ruelle bound, as far as hard-core potentials with an attractive tail are considered, in the case of the new inequality (3.12), applicable to Lennard-Jones type potentials, a direct comparison with the classical bound appears to be quite involved and, in general, model-dependent, since it depends on the ability to get an optimal estimate for the stability constants for given pair potentials. We are however able to produce specific examples of Lennard-Jones type pair potentials for which our bound improves on the classical Ruelle-Penrose bound. This gives us some hope that the new bounds may lead to an improvement on the classical Penrose-Ruelle bound even for general Lennard-Jones type pair potentials. We plan to address such kind of questions in a future paper.

2 Notations and Results

Throughout the paper, if S is a set, then $|S|$ denotes its cardinality. If $n \in \mathbb{N}$ is a natural number then we will denote shortly $[n] = \{1, 2, \dots, n\}$. We also denote $\mathbb{Z}^+ = \mathbb{N} \cup \{0\} = \{0, 1, 2, \dots\}$.

2.1 Continuous particle systems in the grand canonical ensemble

We will focus our attention on a system of classical, identical particles enclosed in a cubic box $\Lambda \subset \mathbb{R}^d$ with volume $|\Lambda|$. We denote by $x_i \in \mathbb{R}^d$ the position d -dimensional vector of the i^{th} particle and by $|x_i|$ its modulus. We assume that there are no particles outside Λ (free boundary conditions) and that particles interact via a pair potential $v(x_i, x_j)$ which, for sake of simplicity, will be assumed to be translational and rotational invariant. Namely we assume that

$$v(x_i, x_j) \equiv V(|x_i - x_j|)$$

with $V(r)$ being a function from $[0, +\infty)$ to $(-\infty, +\infty]$. Given N particles in positions $(x_1, \dots, x_N) \in \Lambda^N$, their (configurational) energy $U(x_1, \dots, x_N)$ is given by

$$U(x_1, \dots, x_N) = \sum_{1 \leq i < j \leq N} V(|x_i - x_j|)$$

Remark. The value $V(r) = +\infty$ for some $r \geq 0$ is allowed. In particular, given a pair potential $V(|x|)$, a pair x_i, x_j is called *incompatible* if $V(|x_i - x_j|) = +\infty$, and we write $x_i \approx x_j$. Otherwise, if $V(|x_i - x_j|) < +\infty$, we say that x_i and x_j are *compatible* and we write $x_i \sim x_j$.

Definition 1 A pair potential $V(|x|)$ is said to be *stable* if there exists $B \geq 0$ such that, for all $N \in \mathbb{N}$ and for all $(x_1, \dots, x_N) \in \mathbb{R}^{dN}$,

$$\sum_{1 \leq i < j \leq N} V(|x_i - x_j|) \geq -BN \quad (2.1)$$

The inf of such B 's is called the *stability constant*.

Definition 2 A pair potential $V(|x|)$ is said to be *tempered* if there exists a constant $r_0 \geq 0$ such that

$$\int_{|x| \geq r_0} |V(|x|)| dx < +\infty \quad (2.2)$$

Definition 3 A pair potential $V(|x|)$ is said to be *admissible* if it is stable and tempered.

Note that a pair potential $V(r)$ satisfying definition 1 is bounded below; namely, by applying (2.1) for the case $N = 2$

$$V(r) \geq -2B \quad \forall r \geq 0$$

Moreover, as a consequence of stability and temperedness it is also easy to check that, for all $\beta > 0$

$$C(\beta) \doteq \int_{\mathbb{R}^d} \left| e^{-\beta V(|x|)} - 1 \right| dx < +\infty \quad (2.3)$$

The grand canonical partition function $\Xi_\Lambda(\beta, \lambda)$ of the system is given by

$$\Xi_\Lambda(\beta, \lambda) = 1 + |\Lambda|\lambda + \sum_{N \geq 2} \frac{\lambda^N}{N!} \int_\Lambda dx_1 \dots \int_\Lambda dx_N e^{-\beta \sum_{1 \leq i < j \leq N} V(|x_i - x_j|)} \quad (2.4)$$

with $\beta > 0$ being the inverse temperature, and $\lambda > 0$ being the fugacity. The pressure of the system is given by

$$P(\beta, \lambda) = \lim_{|\Lambda| \rightarrow \infty} \frac{1}{\beta|\Lambda|} \log \Xi_\Lambda(\beta, \lambda) \quad (2.5)$$

The limit (2.5) is known to exist if the pair potential $V(|x|)$ is admissible, i.e. it is stable and tempered (see e.g. [26], sections 3.3 and 3.4). Moreover, a very well known and old result (see e.g. [16, 17, 18, 26]) states that the factor $\log \Xi_\Lambda(\beta, \lambda)$ can be written in terms of a formal series in powers of λ . Namely,

$$\frac{1}{|\Lambda|} \log \Xi_\Lambda(\beta, \lambda) = \sum_{n \geq 1} C_n(\beta, \Lambda) \lambda^n \quad (2.6)$$

where $C_1(\beta, \Lambda) = 1$ and, for $n \geq 2$,

$$C_n(\beta, \Lambda) = \frac{1}{|\Lambda|} \frac{1}{n!} \int_\Lambda d\mathbf{x}_1 \dots \int_\Lambda d\mathbf{x}_n \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} \left[e^{-\beta V(|x_i - x_j|)} - 1 \right] \quad (2.7)$$

with G_n being the set of all connected graphs with vertex set $[n]$ (here above E_g denotes the edge-set of a graph $g \in G_n$).

The r.h.s. of (2.6) is known as the Mayer series and the term $C_n(\beta, \Lambda)$ defined in (2.7) is the n -th order Mayer coefficient (a.k.a. n -th order connected cluster integral). The dependence on the volume $|\Lambda|$ of the Mayer coefficients $C_n(\beta, \Lambda)$ is, in case of stable and tempered potentials, only marginal, and it is not difficult to show that $|C_n(\beta, \Lambda)|$ admits a bound uniform in Λ and, for every $n \in \mathbb{N}$, the limit

$$C_n(\beta) = \lim_{|\Lambda| \rightarrow \infty} C_n(\beta, \Lambda) \quad (2.8)$$

exists and it is a finite constant (see e.g. [26]). However, it is a completely different story to obtain an upper bound on the (modulus of) n -order Mayer coefficient (2.7) with a good behavior in n (i.e. $C_n(\beta) \sim [C(\beta)]^n$) due to the fact that the cardinality of the set G_n above is not less than $2^{(n-1)(n-2)/2}$. Such kind of bound must be obtained in general by exploiting some hidden cancellations in the factor

$$\left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} \left[e^{-\beta V(|x_i - x_j|)} - 1 \right] \right| \quad (2.9)$$

It is clear that an efficient upper bound for the Mayer coefficients $|C_n(\beta, \Lambda)|$, e.g. of the form $|C_n(\beta, \Lambda)| \leq [C(\beta)]^n$ would immediately yield a lower bound for the convergence radius of the Mayer series of the pressure uniform in the volume.

As remarked in the introduction, as far as admissible potentials (i.e. satisfying condition (2.1) and (2.2)) are concerned, the best rigorous bound on $|C_n(\beta, \Lambda)|$ available in the literature up to now was that obtained by Penrose and Ruelle in 1963.

Theorem 1 (Penrose-Ruelle) *Let $V(|x|)$ be an admissible pair potential. Let B be its stability constant. Then the n -order Mayer coefficient $C_n(\beta, \Lambda)$ defined in (2.7) admits the bound*

$$|C_n(\beta, \Lambda)| \leq e^{2\beta B(n-1)} n^{n-2} \frac{[C(\beta)]^{n-1}}{n!} \quad (2.10)$$

where $C(\beta)$ is the function defined in (2.3).

Consequently, the Mayer series in the r.h.s. of (2.6) converges absolutely, uniformly in Λ for any complex λ inside the disk

$$|\lambda| < \frac{1}{e^{2\beta B+1} C(\beta)} \quad (2.11)$$

As said in the introduction, Brydges and Federbush gave an improvement of the Penrose Ruelle bound as far as absolutely summable pair potentials are considered.

Theorem 2 (Brydges-Federbush) *Let $V(|x|)$ be an admissible and absolutely summable pair potential. Let B be its stability constant and let $\|V\| = \int_{\mathbb{R}^d} V(|x|)dx$. Then the n -order Mayer coefficient $C_n(\beta, \Lambda)$ defined in (2.7) admits the bound*

$$|C_n(\beta, \Lambda)| \leq e^{\beta B(n-1)} n^{n-2} \frac{[\beta \|V\|]^{n-1}}{n!} \quad (2.12)$$

Consequently, the Mayer series in the r.h.s. of (2.6) converges absolutely, uniformly in Λ for any complex λ inside the disk

$$|\lambda| < \frac{1}{e^{\beta B+1} \beta \|V\|} \quad (2.13)$$

It can be easily seen that, as far as absolutely integrable potentials are considered, (2.13) may strongly improve (2.11). Let us consider for example the so-called Morse potential, largely used in simulations of molecular gas models. The Morse potential is defined via the formula

$$V_\rho(|x|) = e^{2\rho(1-|x|)} - 2e^{\rho(1-|x|)}$$

where $\rho > 0$ is a constant. It is known that $V_\rho(|x|)$ is stable for $\rho \geq \ln 16$ (see [26], sec. 3.5.3, exercise 3B). Moreover $V_\rho(|x|)$ is absolutely summable (it is bounded above by $e^{2\rho}$ and bounded below by -1). Choosing $\beta = 1$ for simplicity and, e.g., $\rho = 6$, an easy computation shows that for the Morse potential $C(\beta) \geq \int_{|x| \geq \ln 2/6} |V_{\rho=6}(|x|)| dx \geq 4\pi(182)$, while $\|V_{\rho=6}\| \leq 4\pi(204)$. So if B_6 is the stability constant of $V_{\rho=6}(|x|)$, the ratio between the Penrose-Ruelle bound (2.11) and the Brydges-Federbush bound (2.13) bound for the same convergence radius is smaller than $(1.13)e^{-B_6}$. To have an idea on how small is this ratio (so how much better is the Brydges-Federbush bound with respect to the Penrose-Ruelle bound) for the Morse potential $V_\rho(|x|)$ with $\rho = 6$ one can take a recent upper bound for $B_6 = 38.65$ given in [3]. Using this value we get that, for inverse temperature $\beta = 1$, the Brydges-Federbush bound is at least e^{38} larger than the Penrose-Ruelle bound!

Such a computation indicates (or at least gives hope) that, being able to use the Brydges-Federbush bound also for non absolutely integrable potentials, this could yield improved bounds also in this case. Below we exhibit a class of admissible non absolutely integrable potentials which have an unquestionable relevance in physical applications and for which, as we will see below, the Brydges-Federbush TGI can be implemented.

Definition 4 *An admissible pair potential $V(|x|)$ on \mathbb{R}^d is said to be Ruelle if*

$$V(|x|) = \Phi_1(|x|) + \Phi_2(|x|)$$

where $\Phi_1(|x|)$ is non-negative and tempered and $\Phi_2(|x|)$ is stable and absolutely integrable (i.e. such that $\int_{\mathbb{R}^d} |\Phi_2(|x|)| dx < +\infty$).

Remark. Actually Ruelle considered potentials of the form $V(|x|) = \Phi_1(|x|) + \Phi_2(|x|)$ but required for $\Phi_2(|x|)$ to be, more strongly, a *positive definite* pair potential (i.e. $\Phi_2(|x|)$ is a smooth function with positive Fourier transform). Indeed, any positive-definite potential $\Phi_2(|x|)$ is absolutely summable, because it admits Fourier transform, and stable with stability constant $\Phi_2(0)/2$ (see [26, 10]). Ruelle also conjectured that any stable and tempered potential could always be

written via such a decomposition, but this has been proven to be untrue in [2, 14]. However, the counterexamples found in [2, 14] are absolutely summable stable potentials (so Ruelle according to definition 4) and hence it seems reasonable to conjecture that the class of Ruelle potentials introduced in Definition 4, in which the condition for $\Phi_2(|x|)$ to be *positive-definite* is replaced by the much milder condition for $\Phi_2(|x|)$ to be stable and absolutely summable, actually coincides with the whole class of admissible potentials.

Conjecture 1 *Any stable and tempered pair potential can always be written as a sum of a non-negative potential plus an absolutely summable stable potential.*

The class of potentials introduced in definition 4 appears to be in any case very big and includes many (if not all) physically realistic pair potentials. In particular it contains the so-called Lennard-Jones type potentials.

Definition 5 *An admissible pair potential $V(|x|)$ on \mathbb{R}^d is said to be of Lennard-Jones type if there exist constants w, r_1, r_2 (with $r_1 \leq r_2$) and non-negative monotonic decreasing functions $\xi(|x|), \eta(|x|)$ such that*

$$V(|x|) \begin{cases} \geq \xi(|x|) & \text{if } |x| \leq r_1 \\ \geq -w & \text{if } r_1 \leq |x| \leq r_2 \\ \geq -\eta(|x|) & \text{if } |x| \geq r_2 \end{cases} \quad (2.14)$$

with

$$\int_{|x| \leq r_1} \xi(|x|) dx = +\infty \quad (2.15)$$

and

$$\int_{|x| \geq r_2} \eta(|x|) dx < +\infty \quad (2.16)$$

Indeed, in the appendix of the present paper we will prove the following proposition.

Proposition 1 *Let $V(|x|)$ a Lennard-Jones type pair potential according to Definition 5. Then $V(|x|)$ is Ruelle according to definition 4.*

An interesting subclass of the pair potentials satisfying Definition 4 is the class of hard-core potentials with an attractive tail originally considered by Penrose in [21].

Definition 6 (Penrose pair potential) *An admissible pair potential $V(|x|)$ on \mathbb{R}^d is called Penrose if it has an hard-core, i.e. if there exists a positive constant $a > 0$ such that $V(|x|) = +\infty$ whenever $|x| \leq a$ and $V(|x|) < 0$ whenever $|x| > a$. The constant a is called the hard-core radius of the Penrose pair potential.*

As mentioned in the introduction, Poghosyan and Ueltschi pointed out in [22] that for Penrose potentials the inequality (3.7) proposed in [24, 23] yields new bounds which improve the classical result of Theorem 1.

Theorem 3 *Let $V(|x|)$ be a Penrose potential according to Definition 6. Let B be its stability constant and let a be its hard core radius. Then n -order Mayer coefficient $C_n(\beta, \Lambda)$ defined in (2.7) admits the bound*

$$|C_n(\beta, \Lambda)| \leq e^{\beta B n} n^{n-2} \frac{[C^*(\beta)]^{n-1}}{n!} \quad (2.17)$$

where, if we denote by $W_a(d)$ the volume of the sphere of radius a in d dimensions,

$$C^*(\beta) = W_a(d) + \beta \int_{|x| \geq a} |V(|x|)| dx \quad (2.18)$$

Consequently, the Mayer series converges absolutely for all complex activities λ such that

$$|\lambda| < \frac{1}{e^{\beta B + 1} C^*(\beta)} \quad (2.19)$$

Remark. Formula (2.19) represents an improvement on the classical bound (2.11) for all Penrose potentials with an attractive tail, i.e. those V for which $V(|x|) < 0$ when $|x| > a$ (which are, as a matter of fact, the interesting cases). Indeed, for such V , in formula (2.19) the presence of the factor $e^{\beta B}$ improves (exponentially) the factor $e^{2\beta B}$ of formula (2.11). Moreover $C^*(\beta) < C(\beta)$ for all β since $e^x - 1 > x$ for all $x > 0$. We will give below, for the benefit of the reader, a self-contained proof of Theorem 3.

2.2 Results

The main result of the paper can be summarized by the following theorem.

Theorem 4 *Let $V(|x|) = \Phi_1(|x|) + \Phi_2(|x|)$ be Ruelle potential in the sense of Definition 4 and let \tilde{B} the stability constant of the potential $\Phi_2(|x|)$. Then the n -th order Mayer coefficient $C_n(\beta, \Lambda)$ defined in (2.7) admits the bound*

$$|C_n(\beta, \Lambda)| \leq e^{\beta \tilde{B} n} n^{n-2} \frac{[\tilde{C}(\beta)]^{n-1}}{n!} \quad (2.20)$$

where

$$\tilde{C}(\beta) = \int \left[|e^{-\beta \Phi_1(|x|)} - 1| + \beta |\Phi_2(|x|)| \right] dx \quad (2.21)$$

Consequently, the Mayer series converges absolutely for all complex activities λ such that

$$|\lambda| < \frac{1}{e^{\beta \tilde{B} + 1} \tilde{C}(\beta)} \quad (2.22)$$

Remark. If the Ruelle potential $V(|x|)$ is absolutely integrable, e.g. $V(|x|) = \Phi_2(|x|)$, then (2.22) is the Brydges-Federbush bound (2.13). On the other hand, if $V(|x|)$ is not absolutely integrable then (2.22) is a new bound. In this case however a comparison of bound (2.22) with the original Ruelle-Penrose bound (2.11) appears to be more tricky, since the possible improvement of formula (2.22) with respect to the classical (2.11) is strongly model dependent and, for a fixed potential, could rely on the search of an optimal decomposition $V(|x|) = \Phi_1(|x|) + \Phi_2(|x|)$ providing the as

small as possible constant \tilde{B} and, at the same time, the as small as possible quantity $\tilde{C}(\beta)$. The sharp evaluation of the stability constant of a given potential is quite a hard subject, and it is beyond the scope of this paper. However, it is not difficult to exhibit examples of non absolutely integrable pair potentials (actually the example below is a Lennard-Jones type potential) for which bound (2.21) strongly improves on (2.11). E.g. an example goes as follows. Let $\Phi_2(|x|)$ is an absolutely summable stable potential for which the minimum particle distance r_{\min} in a minimal energy configuration is strictly positive (such kind of potentials do exist: e.g. Morse potentials have $r_{\min} > 0$, see [15]). Let \tilde{B} the stability constant of $\Phi_2(|x|)$. Let now $\xi(r)$ be a positive function such that $\xi(|x|) > \Phi_2(|x|)$ for $|x| < r_{\min}$ and $\int_{|x| < r_{\min}} \xi(|x|) dx = \infty$. Let

$$\Phi_1(|x|) = \begin{cases} \xi(|x|) - \Phi_2(|x|) & \text{if } |x| < r_{\min} \\ 0 & \text{if } |x| \geq r_{\min} \end{cases}$$

Then $V(|x|) = \Phi_1(|x|) + \Phi_2(|x|)$ is a Lennard-Jones type potential given by

$$V(|x|) = \begin{cases} \xi(|x|) & \text{if } |x| < r_{\min} \\ \Phi_2(|x|) & \text{if } |x| \geq r_{\min} \end{cases}$$

By construction, $V(x)$ has the same stability constant \tilde{B} as $\Phi_2(|x|)$. Indeed, minimal energy configurations for $V(|x|)$ are also minimal energy configurations for $\Phi_2(|x|)$ (since $V(|x|) = \Phi_2(|x|)$ for $|x| \geq r_{\min}$) and any energy configuration for $V(|x|)$ in which there are pairs of particles at distance less than r_{\min} has larger energy than the same configuration for $\Phi_2(|x|)$ (because $V(|x|) > \Phi_2(|x|)$ for $|x| < r_{\min}$). Proceeding now as we did in the Morse potential example after Theorem 2, we get that the ratio between the Penrose-Ruelle bound and Brydges-Federbush bound for such $V(|x|)$ with $\beta = 1$ is $e^{-\tilde{B}}(C_1/C_2)$ where $C_1 = \int_{\mathbb{R}^d} |e^{-V(|x|)} - 1| dx$ and $C_2 = \int_{\mathbb{R}^d} \Phi_2(|x|) dx$. Picking Φ_2 and ξ in such a way that $C_1/C_2 = O(1)$ we get, similarly to the case presented in the remark after Theorem 2, that the bound (2.22) is $O(1) \exp \tilde{B}$ times larger than the Penrose-Ruelle bound.

The rest of the paper is organized as follows. In section 3 we will revisit the Brydges-Federbush TGI, introducing the necessary notations, and we will state and prove two technical results, namely Theorem 6 and Theorem 7, which will be the main tools in order to prove Theorems 3 and 4 respectively, whose proofs will be completed in section 4. Finally in the appendix we will prove Proposition 1.

3 Algebraic Brydges-Federbush tree graph identity

3.1 Pair potentials in $[n]$

In this section we present the Brydges-Federbush identity which in turn leads to alternative expressions for the Mayer coefficients defined in (2.7). This alternative expression of the Mayer coefficients is written in terms of a sum over trees rather than connected graphs and, as we will see, this fact permits us to get rid of the combinatorial problem. The Brydges-Federbush identity is essentially algebraic and in order to introduce it we need to give some preliminary notations. We recall that we let $[n] = \{1, 2, \dots, n\}$. We also denote by E_n the set of all unordered pairs in $[n]$ and, in general, if $X \subset [n]$, then E_X will denote the set of all unordered pairs in X .

Definition 7 *An algebraic pair interaction in $[n]$ is a map $V : E_n \rightarrow \mathbb{R} \cup \{+\infty\}$ that associate to any unordered pair in $\{i, j\} \in E_n$ a number V_{ij} (with the convention, $i < j$) with values in $\mathbb{R} \cup \{+\infty\}$*

Definition 8 Let V be an algebraic pair interaction in $[n]$. Let $\{i, j\} \in E_n$. If $V_{ij} = +\infty$ we say that the pair $\{i, j\}$ is incompatible and we write $i \not\sim j$. Otherwise, if $V_{ij} < +\infty$ we say that the pair $\{i, j\}$ is compatible and we write $i \sim j$. A set $X \subset [n]$ is called incompatible if there are $\{i, j\} \in E_X$ such that $i \not\sim j$. Otherwise, if for every $\{i, j\} \in E_X$ we have that $i \sim j$ then X is called a compatible set.

Definition 9 An algebraic pair interaction V in $[n]$ is said to be stable if there exists a constant $B \geq 0$ such that, for all $X \subset [n]$ with $|X| \geq 2$ we have

$$\sum_{\{i,j\} \in E_X} V_{ij} \geq -B|X| \quad (3.1)$$

Observe that, if $V(|x|)$ is a stable pair potential in \mathbb{R}^d in the sense of definition 1 with stability constant (not greater than) B , then for any $n \in \mathbb{N}$ and any n -tuple $(x_1, \dots, x_n) \in \mathbb{R}^{dn}$, the algebraic pair interaction $V_{ij} = V(|x_i - x_j|)$ has stability constant (not greater than) B in the sense of definition 9. Note moreover that we can restrict ourselves to check the condition (3.1) only for those X which do not contain incompatible pairs, otherwise the l.h.s. of (3.1) takes the value $+\infty$.

Definition 10 An algebraic pair interaction V in $[n]$ is said to be repulsive if, $\forall \{i, j\}$

$$V_{ij} \geq 0$$

and V is said to be bounded if, $\forall \{i, j\}$

$$V_{ij} < +\infty$$

Definition 11 An algebraic pair interaction V in $[n]$ is said to be Ruelle-stable if $V = \Phi_1 + \Phi_2$ where Φ_1 is a repulsive pair interaction in $[n]$ and Φ_2 is a bounded and stable pair interaction in $[n]$.

Of course, if $V(|x|) = \Phi_1(|x|) + \Phi_2(|x|)$ is a Ruelle pair potential in \mathbb{R}^d , then for any $n \in \mathbb{N}$ and any n -tuple $(x_1, \dots, x_n) \in \mathbb{R}^{dn}$ the algebraic pair potential V_{ij} in $[n]$ defined by $V_{ij} = V(|x_i - x_j|)$ is Ruelle-stable.

3.2 The Brydges-Federbush tree graph identity

We are now ready to state the (algebraic) Brydges-Federbush tree graph identity. Given an algebraic pair interaction V in $[n]$, consider the factor

$$\sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}} - 1) \quad (3.2)$$

where G_n is the set of connected graph in $[n]$ and, for $g \in G_n$, E_g is the edge set of g . Then the following theorem holds.

Theorem 5 Let V be a bounded algebraic pair interaction in $[n]$, then the following identity holds:

$$\sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}} - 1) = \sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} (-V_{ij}) \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) V_{ij}} \quad (3.3)$$

where

- T_n denotes the set of all trees with vertex set $[n]$ and, for $\tau \in T_n$, E_τ is the edge set of τ ;
- \mathbf{t}_n denotes a set on $n - 1$ interpolating parameters $\mathbf{t}_n \equiv (t_1, \dots, t_{n-1}) \in [0, 1]^{n-1}$;
- the symbol \mathbf{X}_n denotes a set of “increasing” sequences of $n - 1$ subsets, $\mathbf{X}_n \equiv X_1, \dots, X_{n-1}$ such that $\forall i \in [n - 1]$, $X_i \subset [n]$, $X_i \subset X_{i+1}$, $|X_i| = i$ and $X_1 = \{1\}$.
- The factor $\mathbf{t}_n(\{i, j\})$, which depends on \mathbf{X}_n , is defined as

$$\mathbf{t}_n(\{i, j\}) = t_1(\{i, j\}) \dots t_{n-1}(\{i, j\})$$

with, for $s \in [n - 1]$ and $\{i, j\} \in E_n$,

$$t_s(\{i, j\}) = \begin{cases} t_s \in [0, 1] & \text{if } i \in X_s \text{ and } j \notin X_s \text{ or viceversa} \\ 1 & \text{otherwise} \end{cases}$$

- The measure $\mu_\tau(\mathbf{t}_n, \mathbf{X}_n)$ is the following probability measure

$$\int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n)[\dots] = \int_0^1 dt_1 \dots \int_0^1 dt_{n-1} \sum_{\substack{\mathbf{X}_n \\ \text{compatible with } \tau}} t_1^{b_1-1} \dots t_{n-1}^{b_{n-1}-1}[\dots]$$

where $\mathbf{X}_n = (X_1, \dots, X_{n-1})$ compatible with τ means that $\forall i \in [n - 1]$, X_i contains exactly $i - 1$ edges of τ and b_i is the number of edges of τ which have one vertex in X_i and the other one in $[n] \setminus X_i$.

We refer the reader to references [5] and [25] for a detailed proof.

Remark. The hypothesis that V has to be a bounded pair interaction is necessary to give meaning to the r.h.s. of (3.3), in particular to the factor $\prod_{\{i,j\} \in \tau} (-V_{ij})$. However Theorem 5 immediately implies the following corollary.

Corollary 1 *Let V be a pair interaction in $[n]$ not necessarily bounded (i.e. $V_{ij} = +\infty$ for some $\{i, j\} \in E_n$ is allowed). Then following identity holds:*

$$\sum_{g \in G_n} \prod_{\{i,j\} \in g} (e^{-V_{ij}} - 1) = \lim_{H \rightarrow +\infty} \sum_{\tau \in T_n} \prod_{\{i,j\} \in \tau} (-V_{ij}^H) \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) V_{ij}^H} \quad (3.4)$$

where V^H is the bounded pair potential on $[n]$ given by

$$V_{ij}^H = \begin{cases} H & \text{if } V_{ij} = +\infty \\ V_{ij} & \text{otherwise} \end{cases} \quad (3.5)$$

Proof. Indeed, by theorem 3.3 we have that, for all $H \in \mathbb{R}$,

$$\sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} (-V_{ij}^H) \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) V_{ij}^H} = \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}^H} - 1)$$

and

$$\sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}} - 1) = \lim_{H \rightarrow +\infty} \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}^H} - 1)$$

□

We finally conclude this section by recalling two lemmas which will be used below. We refer again the reader to references [5] and [25] for their proofs.

Lemma 1 *Let V be a bounded algebraic pair potential in $[n]$, then for any $\tau \in T_n$ it holds the identity*

$$\prod_{\{i,j\} \in E_\tau} |e^{-V_{ij}} - 1| = \prod_{\{i,j\} \in E_\tau} |V_{ij}| \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{\{i,j\} \in E_\tau} \mathbf{t}_n(\{i,j\}) V_{ij}} \quad (3.6)$$

Lemma 2 *Let V_{ij} a stable algebraic pair interaction in $[n]$ with stability constant B , then, for all X_1, \dots, X_{n-1} and all $(t_1, t_2, \dots, t_{n-1}) \in [0, 1]^{n-1}$*

$$\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i, j\}) V_{ij} \geq -nB$$

3.3 New Tree graph inequalities from Brydges-Federbush TGI

We are now ready to enunciate the two main technical results derived from the algebraic Brydges-Federbush tree graph identity. The first of them (Theorem 6 below) has been originally proved in [23, 24]. The second result (Theorem 7 below) is, as far as we know, a new result. Theorem 6 will be used later to obtain improved bounds (respect to the classical bounds (2.10)-(2.11)) for the convergence radius of the Mayer expansion in systems of particles interacting through a Penrose pair potential according to Definition 6. Theorem 7 will be used later to obtain new bounds, alternative to the classical ones (2.10) and (2.11), in systems of particles interacting through a Ruelle pair potential according to Definition 4.

Theorem 6 *Let V be a stable algebraic pair interaction in $[n]$ with stability constant B , then the following inequality holds:*

$$\left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}} - 1) \right| \leq e^{nB} \sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} F_{ij} \quad (3.7)$$

where

$$F_{ij} = \begin{cases} |e^{-V_{ij}} - 1| \equiv 1 & \text{if } V_{ij} = +\infty \\ |V_{ij}| & \text{otherwise} \end{cases} \quad (3.8)$$

Proof. By theorem 3.3 and corollary 1 we have that

$$\left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}} - 1) \right| = \lim_{H \rightarrow \infty} \left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}^H} - 1) \right| =$$

$$\begin{aligned}
&= \lim_{H \rightarrow +\infty} \left| \sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} (-V_{ij}^H) \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) V_{ij}^H} \right| \leq \\
&\leq \lim_{H \rightarrow +\infty} \sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} |V_{ij}^H| \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) V_{ij}^H} \doteq \lim_{H \rightarrow +\infty} \sum_{\tau \in T_n} w_\tau^H
\end{aligned}$$

where

$$w_\tau^H = \prod_{\{i,j\} \in E_\tau} |V_{ij}^H| \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) V_{ij}^H}$$

Observe now that, for any tree $\tau \in T_n$, the edge set E_τ is naturally partitioned into two disjoint sets E_τ^H and $E_\tau \setminus E_\tau^H$ where

$$E_\tau^H = \{\{i,j\} \subset E_\tau : i \not\sim j\}$$

So, by definition (3.5)

$$w_\tau^H = H^{|E_\tau^H|} \prod_{\{i,j\} \in E_\tau \setminus E_\tau^H} |V_{ij}| \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) V_{ij}^H}$$

Now, we can rewrite

$$\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) V_{ij}^H = \sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) U_{ij}^{(1-\varepsilon)H} + \sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) V_{ij}^{\varepsilon H}$$

where $\varepsilon > 0$ and

$$U_{ij}^{(1-\varepsilon)H} = \begin{cases} (1-\varepsilon)H & \text{if } i \sim j \\ 0 & \text{otherwise} \end{cases}$$

and

$$V_{ij}^{\varepsilon H} = \begin{cases} \varepsilon H & \text{if } i \sim j \\ V_{ij} & \text{otherwise} \end{cases}$$

The algebraic pair interaction $V^{\varepsilon H}$ in $[n]$, when H is taken sufficiently large, is stable with the stability constant equal to that of the algebraic pair interaction V in the sense of definition 9. Namely, there exists an $H_0 > 0$ (which depends on V and n) such that for all $H \geq H_0$

$$\sum_{\{i,j\} \in E_X} V_{ij}^{\varepsilon H} \geq -B|X|$$

for all $X \subset [n]$. So, by proposition 2 we have

$$\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) V_{ij}^{\varepsilon H} \geq -nB$$

and thus we can bound, for $H \geq H_0$

$$w_\tau^H \leq e^{Bn} \left[\prod_{\{i,j\} \in E_\tau \setminus E_\tau^H} |V_{ij}| \right] H^{|E_\tau^H|} \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) U_{ij}^{(1-\varepsilon)H}} \quad (3.9)$$

On the other hand the potential $U_{ij}^{(1-\varepsilon)H}$ is non negative, so

$$\begin{aligned}
& \sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i, j\}) U_{ij}^{(1-\varepsilon)H} \geq \sum_{\{i, j\} \subset E_\tau^H} \mathbf{t}_n(\{i, j\}) U_{ij}^{(1-\varepsilon)H} = \\
& = \sum_{\{i, j\} \subset E_\tau^H} \mathbf{t}_n(\{i, j\}) (1 - \varepsilon)H + \eta \sum_{\{i, j\} \subset E_\tau \setminus E_\tau^H} \mathbf{t}_n(\{i, j\}) - \eta \sum_{\{i, j\} \subset E_\tau \setminus E_\tau^H} \mathbf{t}_n(\{i, j\}) \geq \\
& \geq \sum_{\{i, j\} \subset E_\tau^H} \mathbf{t}_n(\{i, j\}) (1 - \varepsilon)H + \sum_{\{i, j\} \subset E_\tau \setminus E_\tau^H} \mathbf{t}_n(\{i, j\}) \eta - |E_\tau \setminus E_\tau^H| \eta \\
& \geq \sum_{\{i, j\} \subset E_\tau} \mathbf{t}_n(\{i, j\}) V_{ij}^\tau - \eta |E_\tau \setminus E_\tau^H|
\end{aligned} \tag{3.10}$$

where V_{ij}^τ is the positive (H dependent) pair potential given by

$$V_{ij}^\tau = \begin{cases} (1 - \varepsilon)H & \text{if } \{i, j\} \in E_\tau^H \\ \eta & \text{if } \{i, j\} \in E_\tau \setminus E_\tau^H \end{cases} \tag{3.11}$$

Plugging (3.11) into (3.10) and observing that, by definition (3.11), we can write

$$H^{|E_\tau^H|} = \left[\frac{1}{\eta} \right]^{|E_\tau \setminus E_\tau^H|} \left[\frac{1}{1 - \varepsilon} \right]^{|E_\tau^H|} \prod_{\{i, j\} \in E_\tau} V_{ij}^\tau$$

we arrive at

$$\begin{aligned}
w_H^\tau & \leq e^{nB} \left[\prod_{\{i, j\} \in E_\tau \setminus E_\tau^H} |V_{ij}| \right] \times \\
& \times \left[\frac{e\eta}{\eta} \right]^{|E_\tau \setminus E_\tau^H|} \left[\frac{1}{1 - \varepsilon} \right]^{|E_\tau^H|} \times \prod_{\{i, j\} \in E_\tau} V_{ij}^\tau \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{\{i, j\} \subset E_\tau} \mathbf{t}_n(\{i, j\}) V_{ij}^\tau}
\end{aligned}$$

Using now Lemma 1, i.e. formula (3.6) we have that

$$\begin{aligned}
& \prod_{\{i, j\} \in E_\tau} V_{ij}^\tau \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{\{i, j\} \subset E_\tau} \mathbf{t}_n(\{i, j\}) V_{ij}^\tau} = \prod_{\{i, j\} \in E_\tau} \left| e^{-V_{ij}^\tau} - 1 \right| = \\
& = \prod_{\{i, j\} \in E_\tau^H} \left| e^{-U_{ij}^{(1-\varepsilon)H}} - 1 \right| \left| e^{-\eta} - 1 \right|^{|E_\tau \setminus E_\tau^H|} \leq \prod_{\{i, j\} \in E_\tau^H} |e^{-V_{ij}} - 1| \left| e^{-\eta} - 1 \right|^{|E_\tau \setminus E_\tau^H|}
\end{aligned}$$

where in the last line we have used that $U_{ij}^{(1-\varepsilon)H} < V_{ij}$ for all $H > 0$ and for all $\{i, j\} \subset [n]$ such that $i \asymp j$. Thus we get, for $H \geq H_0$

$$w_H^\tau \leq e^{nB} \left[\prod_{\{i, j\} \in E_\tau \setminus E_\tau^H} |V_{ij}| \right] \times$$

$$\begin{aligned}
& \times \left[\frac{e^\eta |e^{-\eta} - 1|}{\eta} \right]^{|E_\tau \setminus E_\tau^H|} \left[\frac{1}{1 - \varepsilon} \right]^{|E_\tau^H|} \times \prod_{\{i,j\} \in E_\tau^H} |e^{-V_{ij}} - 1| = \\
& = e^{nB} \left[\prod_{\{i,j\} \in E_\tau \setminus E_\tau^H} \frac{(e^\eta - 1)}{\eta} |V_{ij}| \right] \prod_{\{i,j\} \in E_\tau^H} \frac{1}{1 - \varepsilon} |e^{-V_{ij}} - 1| =
\end{aligned}$$

Hence, since η and ε can be taken as small as we please, we get finally

$$w_H^\tau \leq e^{nB} \prod_{\{i,j\} \in E_\tau} F_{ij}$$

where F_{ij} is precisely the function defined in (3.8). \square

Theorem 7 *Let $V = \Phi^1 + \Phi^2$ be a Ruelle algebraic pair interaction in $[n]$ (in the sense of Definition 4) with Φ^1 non-negative and Φ^2 stable. Let B_0 the stability constants associated to Φ_2 . Then the following inequality holds:*

$$\left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}} - 1) \right| \leq e^{nB_0} \sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} \left[|e^{-\Phi_{ij}^1} - 1| + |\Phi_{ij}^2| \right] \quad (3.12)$$

Proof. First observe that by definition Φ^2 is a bounded potential, so if for some $\{i, j\}$ we have that $V_{ij} = +\infty$ then $\Phi_{ij}^1 = +\infty$ while $\Phi_{ij}^2 < +\infty$. Hence we define

$$\Phi_{ij}^{1,H} = \begin{cases} H & \text{if } \Phi_{ij}^1 = +\infty \\ \Phi_{ij}^1 & \text{otherwise} \end{cases}$$

and

$$V_{ij}^H = \Phi_{ij}^{1,H} + \Phi_{ij}^2$$

Then by theorem 5 and corollary 1 we have that

$$\begin{aligned}
& \left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}} - 1) \right| = \lim_{H \rightarrow +\infty} \left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}^H} - 1) \right| = \\
& = \lim_{H \rightarrow +\infty} \left| \sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} (-V_{ij}^H) \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) V_{ij}^H} \right| \leq \\
& \leq \lim_{H \rightarrow +\infty} \sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} |V_{ij}^H| \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) V_{ij}^H} \leq \\
& \leq \lim_{H \rightarrow +\infty} \sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} \left[|\Phi_{ij}^{1,H}| + |\Phi_{ij}^2| \right] \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) [\Phi_{ij}^{1,H} + \Phi_{ij}^2]} \leq \\
& \leq e^{nB_0} \lim_{H \rightarrow +\infty} \sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} \left[|\Phi_{ij}^{1,H}| + |\Phi_{ij}^2| \right] \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\}) \Phi_{ij}^{1,H}}
\end{aligned}$$

where in the last line we have used the stability condition on the factor $e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\})\Phi_{ij}^2}$. Let us now define, for a fixed $\tau \in T_n$ a variable σ with values in $\{1, 2\}$ associated to each edge of E_τ , and for each edge $\{i, j\} \in E_\tau$ the numbers

$$\Phi_{ij}^\sigma = \begin{cases} |\Phi_{ij}^{1,H}| & \text{if } \sigma = 1 \\ |\Phi_{ij}^2| & \text{if } \sigma = 2 \end{cases}$$

Let Σ_τ be the set of all functions $\sigma : E_\tau \rightarrow \{1, 2\}$, then clearly

$$\prod_{\{i,j\} \in E_\tau} \left[|\Phi_{ij}^{1,H}| + |\Phi_{ij}^2| \right] = \sum_{\sigma \in \Sigma_\tau} \prod_{\{i,j\} \in E_\tau} \Phi_{ij}^\sigma$$

Then we can write

$$\begin{aligned} & \left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}} - 1) \right| \leq \\ & \leq e^{nB_0} \lim_{H \rightarrow +\infty} \sum_{\tau \in T_n} \sum_{\sigma \in \Sigma_\tau} \prod_{\{i,j\} \in E_\tau} \Phi_{ij}^\sigma \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\})\Phi_{ij}^{1,H}} \\ & \doteq e^{nB_0} \lim_{H \rightarrow +\infty} \sum_{\tau \in T_n} \sum_{\sigma \in \Sigma_\tau} w_{\tau,\sigma}^H \end{aligned} \quad (3.13)$$

where

$$w_{\tau,\sigma}^H = \prod_{\{i,j\} \in E_\tau} \Phi_{ij}^\sigma \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\})\Phi_{ij}^{1,H}}$$

Observe now that, for any tree $\tau \in T_n$ and any fixed $\sigma \in \Sigma_\tau$, the edge set E_τ is naturally partitioned into two disjoint sets E_τ^1 and $E_\tau^2 = E_\tau \setminus E_\tau^1$ where

$$E_\tau^1 = \{\{i, j\} \in E_\tau : \sigma(\{i, j\}) = 1\}$$

In other words E_τ^1 is formed with those edges $\{i, j\}$ of τ such that $\Phi_{ij}^\sigma = |\Phi_{ij}^{1,H}|$ and $E_\tau \setminus E_\tau^1$ is formed with those edges $\{i, j\}$ of τ such that $\Phi_{ij}^\sigma = |\Phi_{ij}^2|$. So

$$w_{\tau,\sigma}^H = \prod_{\{i,j\} \in E_\tau^1} |\Phi_{ij}^{1,H}| \prod_{\{i,j\} \in E_\tau^2} |\Phi_{ij}^2| \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i,j\})\Phi_{ij}^{1,H}} \quad (3.14)$$

The potential $\Phi_{ij}^{1,H}$ is non negative, so

$$\begin{aligned} & \sum_{1 \leq i < j \leq n} \mathbf{t}_n(\{i, j\})\Phi_{ij}^{1,H} \geq \sum_{\{i,j\} \in E_\tau^1} \mathbf{t}_n(\{i, j\})\Phi_{ij}^{1,H} = \\ & = \sum_{\{i,j\} \in E_\tau^1} \mathbf{t}_n(\{i, j\})\Phi_{ij}^{1,H} + \eta \sum_{\{i,j\} \in E_\tau \setminus E_\tau^1} \mathbf{t}_n(\{i, j\}) - \eta \sum_{\{i,j\} \in E_\tau \setminus E_\tau^1} \mathbf{t}_n(\{i, j\}) \geq \\ & \geq \sum_{\{i,j\} \in E_\tau^1} \mathbf{t}_n(\{i, j\})\Phi_{ij}^{1,H} + \sum_{\{i,j\} \in E_\tau \setminus E_\tau^1} \mathbf{t}_n(\{i, j\})\eta - |E_\tau^2|\eta \end{aligned}$$

$$\geq \sum_{\{i,j\} \in E_\tau} \mathbf{t}_n(\{i,j\}) V_{ij}^\tau - \eta |E_\tau^2| \quad (3.15)$$

where V_{ij}^τ is the positive (H dependent) pair potential given by

$$V_{ij}^\tau = \begin{cases} \Phi_{ij}^{1,H} & \text{if } \{i,j\} \in E_\tau^1 \\ \eta & \text{if } \{i,j\} \in E_\tau^2 \end{cases} \quad (3.16)$$

Plugging (3.15) into (3.14), we can write

$$w_{\tau,\sigma}^H \leq \left[\frac{e^\eta}{\eta} \right]^{|E_\tau^2|} \prod_{\{i,j\} \in E_\tau^2} |\Phi_{ij}^2| \prod_{\{i,j\} \in E_\tau} V_{ij}^\tau \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{\{i,j\} \in E_\tau} \mathbf{t}_n(\{i,j\}) V_{ij}^\tau}$$

Using now Lemma 1, i.e. formula (3.6), we have that

$$\begin{aligned} \prod_{\{i,j\} \in E_\tau} V_{ij}^\tau \int d\mu_\tau(\mathbf{t}_n, \mathbf{X}_n) e^{-\sum_{\{i,j\} \in E_\tau} \mathbf{t}_n(\{i,j\}) V_{ij}^\tau} &= \prod_{\{i,j\} \in E_\tau} \left| e^{-V_{ij}^\tau} - 1 \right| = \\ &= \prod_{\{i,j\} \in E_\tau^1} \left| e^{-\Phi_{ij}^{1,H}} - 1 \right| \left| e^{-\eta} - 1 \right|^{|E_\tau^2|} \end{aligned}$$

Thus we get,

$$w_{\tau,\sigma}^H \leq \left[\prod_{\{i,j\} \in E_\tau^2} \frac{(e^\eta - 1)}{\eta} |\Phi_{ij}^2| \right] \prod_{\{i,j\} \in E_\tau^1} \left| e^{-\Phi_{ij}^{1,H}} - 1 \right| =$$

Hence, since η can be taken as small as we please, we get finally

$$w_{\tau,\sigma}^H \leq \left[\prod_{\{i,j\} \in E_\tau^2} |\Phi_{ij}^2| \right] \prod_{\{i,j\} \in E_\tau^1} \left| e^{-\Phi_{ij}^{1,H}} - 1 \right| \quad (3.17)$$

Plugging (3.17) into (3.13) we get

$$\begin{aligned} &\left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} (e^{-V_{ij}} - 1) \right| \leq \\ &\leq e^{nB_0} \lim_{H \rightarrow +\infty} \sum_{\tau \in T_n} \sum_{\sigma \in \Sigma_\tau} \left[\prod_{\{i,j\} \in E_\tau^2} |\Phi_{ij}^2| \right] \prod_{\{i,j\} \in E_\tau^1} \left| e^{-\Phi_{ij}^{1,H}} - 1 \right| = \\ &= e^{nB_0} \sum_{\tau \in T_n} \sum_{\sigma \in \Sigma_\tau} \left[\prod_{\{i,j\} \in E_\tau^2} |\Phi_{ij}^2| \right] \prod_{\{i,j\} \in E_\tau^1} \left| e^{-\Phi_{ij}^1} - 1 \right| = \\ &= e^{nB_0} \sum_{\tau \in T_n} \prod_{\{i,j\} \in E_\tau} \left[|\Phi_{ij}^2| + \left| e^{-\Phi_{ij}^1} - 1 \right| \right] \end{aligned}$$

□

4 Proof of Theorems 3 and 4

We can now use Theorems 6 and 7 straightforwardly to obtain the new bounds for the Mayer coefficient and consequently the Mayer series radius of convergence as far as Penrose potentials and Ruelle Potentials are concerned.

4.1 Proof of Theorem 3

Let $V(|x|)$ be Penrose pair potential according to Definition 6 and let B be its stability constant. Then, for any $n \in \mathbb{N}$ and $(x_1, \dots, x_n) \in \mathbb{R}^{dn}$, $V_{ij} = \beta V(|x_i - x_j|)$ (with $1 \leq i < j \leq n$) is a stable algebraic potential in $[n]$ with stability constant βB , according to definitions 7 and 9. Therefore we can use Theorem 6 to get a bound on the n -order coefficient $C_n(\beta, \Lambda)$, defined in (2.7), of the Mayer series of the system of particles interacting via the pair potential $V(|x|)$. The bound goes as follows.

$$\begin{aligned} |C_n(\beta, \Lambda)| &\leq \frac{1}{|\Lambda|} \frac{1}{n!} \int_{\Lambda} dx_1 \dots \int_{\Lambda} dx_n \left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} [e^{-\beta V(|x_i - x_j|)} - 1] \right| \leq \\ &\leq \frac{1}{|\Lambda|} \frac{1}{n!} e^{n\beta B} \sum_{\tau \in T_n} \int_{\Lambda} dx_1 \dots \int_{\Lambda} dx_n \prod_{\{i,j\} \in E_{\tau}} F(|x_i - x_j|) \end{aligned} \quad (4.1)$$

where

$$F_{\beta}(|x_i - x_j|) = \begin{cases} |e^{-\beta V(|x_i - x_j|)} - 1| \equiv 1 & \text{if } V(|x_i - x_j|) = +\infty \\ \beta |V(|x_i - x_j|)| & \text{otherwise} \end{cases}$$

Let now a be the hard-core radius of the potential $V(|x|)$. Then, recalling (2.18), we have

$$\int_{\mathbb{R}^d} F(|x|) dx = \int_{|x| \leq a} 1 dx + \beta \int_{|x| \geq a} |V(|x|)| dx = C^*(\beta)$$

Moreover, using standard observations in cluster expansions, we have that, for any tree $\tau \in T_n$

$$\int_{\Lambda} dx_1 \dots \int_{\Lambda} dx_n \prod_{\{i,j\} \in E_{\tau}} F(|x_i - x_j|) \leq |\Lambda| \left(\int_{\mathbb{R}^d} F(|x|) dx \right)^{n-1} = |\Lambda| [C^*(\beta)]^{n-1} \quad (4.2)$$

Plugging now (4.2) into (4.1) and recalling that $\sum_{\tau \in T_n} 1 = n^{n-2}$, we get the desired bound (2.17). \square

4.2 Proof of Theorem 4

Proceeding similarly as above, let now $V(|x|) = \Phi_1(|x|) + \Phi_2(|x|)$ denote a Ruelle pair potential according to Definition 4 and let \tilde{B} be the stability constant of the potential $\Phi_2(|x|)$. Then, for any $n \in \mathbb{N}$ and $(x_1, \dots, x_n) \in \mathbb{R}^{dn}$, $V_{ij} = \beta V(|x_i - x_j|)$ (with $1 \leq i < j \leq n$) is a Ruelle-stable algebraic potential in $[n]$ according to Definition 11, such that

$$V_{ij} = \Phi_{ij}^1 + \Phi_{ij}^2 \quad \text{with} \quad \Phi_{ij}^1 = \beta \Phi_1(|x_i - x_j|) \quad \text{and} \quad \Phi_{ij}^2 = \beta \Phi_2(|x_i - x_j|)$$

Moreover Φ^2 has stability constant $\beta\tilde{B}$. We can now use Theorem 7 to bound the n -order Mayer coefficient as follows.

$$\begin{aligned} |C_n(\beta, \Lambda)| &\leq \frac{1}{|\Lambda|} \frac{1}{n!} \int_{\Lambda} dx_1 \dots \int_{\Lambda} dx_n \left| \sum_{g \in G_n} \prod_{\{i,j\} \in E_g} \left[e^{-\beta V(|x_i - x_j|)} - 1 \right] \right| \leq \\ &\leq \frac{1}{|\Lambda|} \frac{1}{n!} e^{n\beta\tilde{B}} \sum_{\tau \in T_n} \int_{\Lambda} dx_1 \dots \int_{\Lambda} dx_n \prod_{\{i,j\} \in E_{\tau}} \left[|e^{-\beta\Phi_1(|x_i - x_j|)} - 1| + |\beta\Phi_2(|x_i - x_j|)| \right] \end{aligned} \quad (4.3)$$

Recalling now (2.21) and proceeding in a completely analogous manner as we did in the proof of Theorem 3, we have that, for any tree $\tau \in T_n$

$$\begin{aligned} &\int_{\Lambda} dx_1 \dots \int_{\Lambda} dx_n \prod_{\{i,j\} \in E_{\tau}} \left[|e^{-\beta\Phi_1(|x_i - x_j|)} - 1| + |\beta\Phi_2(|x_i - x_j|)| \right] \leq \\ &\leq |\Lambda| \left(\int_{\mathbb{R}^d} \left[|e^{-\beta\Phi_1(|x|)} - 1| + |\beta\Phi_2(|x|)| \right] dx \right)^{n-1} = |\Lambda| \left[\tilde{C}(\beta) \right]^{n-1} \end{aligned} \quad (4.4)$$

Plugging now (4.4) into (4.3) and using again that $\sum_{\tau \in T_n} 1 = n^{n-2}$, we get the bound (2.20). \square

Appendix: proof of Proposition 1

Let $V(|x|)$ be a Lennard-Jones type potential according to Definition 1, let $a > 0$ and let

$$V_a(|x|) = \begin{cases} V(|x|) & \text{if } |x| \geq a \\ V(a) & \text{if } |x| < a \end{cases} \quad (A.1)$$

We will first prove that, for sufficiently small $a \in (0, r_1)$, the potential $V_a(|x|)$ defined in (A.1) is stable by showing that it can be written as a sum of a positive potential plus a positive-definite potential (see [26, 10] and see also remark after definition 4). We basically follow the strategy adopted by Fisher and Ruelle [9] who showed the same in case of Lennard-Jones type potentials. The proof is developed in three steps.

1. We first construct a bounded monotonic decreasing tempered and non-negative function $\eta_3(|x|)$ such that

$$V_a(|x|) \geq -\eta_3(|x|) \quad (A.2)$$

and such that the Fourier transform $\hat{\eta}_3(p)$ of $\eta_3(r)$ (which exists since η_3 is absolutely integrable) is bounded as

$$|\hat{\eta}_3(p)| \leq \frac{C_1}{(|ap|^2 + 1)^d} \quad (A.3)$$

where C_1 is a constant and a is the same constant appearing in (A.1). Recall that, since $\eta_3(|x|)$ is a radial function in \mathbb{R}^d , then its Fourier transform is also radial and moreover $\hat{\eta}_3(p)$ is real.

2. We then construct a bounded monotonic compact support (hence tempered) non negative function $\xi_1(|x|)$ such that

$$\xi_1(|x|) = \begin{cases} \leq V_a(|x|) & \text{if } |x| \leq r_1 \\ 0 & \text{otherwise} \end{cases} \quad (\text{A.4})$$

and the Fourier transform $\hat{\xi}_1(p)$ of $\xi_1(|x|)$ (which exists since $\xi_1(|x|)$ is absolutely integrable) is positive and bounded as

$$\hat{\xi}_1(p) \geq \frac{C_2}{(|ap|^2 + 1)^d} \quad (\text{A.5})$$

with C_2 constant and a is the same constant appearing in (A.1).

3. Once functions $\eta_3(|x|)$ and $\xi_1(|x|)$ with the properties (A.2), (A.3), (A.4), (A.5) have been constructed we write

$$V_a(|x|) = \Psi_1(|x|) + \Psi_2(|x|)$$

with

$$\Psi_1(|x|) = V_a(|x|) + \eta_3(|x|) - \xi_1(|x|)$$

and

$$\Psi_2(|x|) = \xi_1(|x|) - \eta_3(|x|)$$

Note that both $\Psi_1(|x|)$ and $\Psi_2(|x|)$ are tempered since they are sum of tempered functions (recall that $V(|x|)$ is assumed tempered by hypothesis). Moreover, by (A.2) and (A.4) we have immediately that $\Psi_1(|x|) \geq 0$ for all $|x| \geq 0$. Finally, by (A.3) and (A.5) we have that $\Psi_2(|x|)$ has non negative fourier transform and thus is positive definite.

1. *Construction of the function $\eta_3(|x|)$.* Let us construct the function $\eta_3(r)$ with properties (A.2) and (A.3). We first pose

$$\eta_1(|x|) = \begin{cases} w & \text{if } |x| \leq r_2 \\ \eta(|x|) & \text{if } |x| > r_2 \end{cases}$$

So that, for all $|x| \geq 0$, we have that

$$V_a(|x|) \geq -\eta_1(|x|) \quad (\text{A.6})$$

Then we, letting $a \in (0, r_1)$, define

$$\eta_2(|x|) = \begin{cases} w & \text{if } |x| \leq a \\ \eta_1(|x| - a) & \text{if } |x| \geq a \end{cases} \quad (\text{A.7})$$

Of course, by construction, $\eta_1(|x|)$ and $\eta_2(|x|)$ are absolutely summable functions (since $\eta(|x|)$ is tempered). Indeed, if we let $H = \int_{|x| \geq r_2} \eta(|x|) dx$. Then

$$\|\eta_1\|_1 = \frac{\pi^{\frac{d}{2}} r_2^d}{\Gamma(\frac{d}{2} + 1)} w + H$$

and

$$\|\eta_2\|_1 = \frac{\pi^{\frac{d}{2}}(r_2 + a)^d}{\Gamma(\frac{d}{2} + 1)}w + H \leq \frac{\pi^{\frac{d}{2}}(r_2 + r_1)^d}{\Gamma(\frac{d}{2} + 1)}w + H$$

Moreover we have that

$$\eta_2(|x'|) \geq \eta_1(|x|) \quad \text{if } ||x| - |x'|| \leq a \quad (\text{A.8})$$

Now take a non-negative function $\psi(|x|)$ such that $\psi(|x|) = 0$ whenever $|x| > 1$ and such that

$$\int_{\mathbb{R}^d} \psi(|x|)dx = 1 \quad (\text{A.9})$$

It is always possible to choose this function ψ in such a way that it has continuous derivatives of all orders in such a way that its Fourier transform decays at large distances faster than any inverse polynomial. In other words it is always possible to find a (universal) constant C' such that, if $\tilde{\psi}(p) = \int \psi(|x|)e^{ip \cdot x}dx$ is the Fourier transform of $\psi(|x|)$, we have that

$$|\tilde{\psi}(p)| \leq \frac{C'}{(1 + p^2)^d}$$

Note that $\tilde{\psi}(p)$ is real and radial. Let now

$$\psi_a(|x|) = \frac{1}{a^d} \psi\left(\frac{|x|}{a}\right)$$

We have clearly that

$$\int_{\mathbb{R}^d} \psi_a(|x|)dx = 1 \quad (\text{A.10})$$

and $\psi_a(|x|) = 0$ if $|x| > a$. Define now

$$\eta_3(|x|) = \int \psi_a(|x - x'|)\eta_2(x')dx'$$

Due to (A.8) and to the fact that $\psi_a(|x|) = 0$ if $|x| > a$, we have that

$$\eta_3(|x|) = \int \psi_a(|x - x'|)\eta_2(|x'|)dx' \geq \int \psi_a(|x - x'|)\eta_1(|x|)dx' = \eta_1(|x|)$$

and hence, due to (A.6) we have that

$$V_a(|x|) \geq -\eta_3(|x|)$$

Moreover $\eta_3(|x|)$ is absolutely integrable (since, by (A.9)), $\|\eta_3\|_1 = \|\eta_2\|_1$ and its Fourier transform is

$$\tilde{\eta}_3(p) = \tilde{\eta}_2(p)\tilde{\psi}_a(p) = \tilde{\eta}_2(p)\tilde{\psi}(ap)$$

So that

$$|\tilde{\eta}_3(p)| \leq \|\eta_2\|_1 |\tilde{\psi}(ap)| \leq \frac{\left[\frac{\pi^{\frac{d}{2}}(r_2 + r_1)^d}{\Gamma(\frac{d}{2} + 1)}w + H \right] C'}{[1 + (ap^2)^d]}$$

2. *Construction of the function $\xi_1(r)$.* Take a radial function $\chi(|x|)$ (not identically zero) which is non negative, continuous and vanishes for $|x| \geq \frac{1}{2}$. Let now

$$\chi_1(|x|) = \int dx' \chi(|x - x'|) \chi(|x'|)$$

By construction $\chi_1(|x|)$ is continuous non negative and vanishes for $|x| \geq 1$. Moreover the Fourier transform $\tilde{\chi}_1(p)$ of $\chi_1(|x|)$ is non negative (since it is the square of the Fourier transform of $\chi(|x|)$ which is radial and real) and it is non zero in some neighbor of $p = 0$ (since $\tilde{\chi}_1(p = 0) > 0$). Consider now

$$\chi_2(|x|) = \chi_1(|x|) \Psi(|x|) \tag{A.11}$$

where

$$\Psi(|x|) = \int dp \frac{e^{ip \cdot x}}{(p^2 + 1)^d}$$

Then $\chi_2(|x|)$ is non negative (since the integral in (A.11) is the modified Bessel function of the third kind) and vanishes for $r \geq 1$. Moreover its Fourier transform is

$$\tilde{\chi}_2(p) = \int dp' \frac{\tilde{\chi}_1(p')}{[(p - p')^2 + 1]^d} \geq \frac{C''}{[p^2 + 1]^d}$$

where in the last line we have used the fact that $\tilde{\chi}_1(p')$ is strictly positive at $p = 0$ and it is continuous. Let now $K = \max\{\chi_2(x)\}$ and define

$$\chi_3(|x|) = \frac{1}{K} \chi_2(|x|)$$

Then $\chi_3(|x|)$ vanishes for $|x| \geq 1$, and $\chi_3(|x|) \leq 1$ when $|x| < 1$. Moreover its Fourier transform $\tilde{\chi}_3(p)$ is such that

$$\tilde{\chi}_3(p) \geq \frac{C^*}{[p^2 + 1]^d}$$

where

$$C^* = \frac{C''}{K}$$

Let now, for $a \in (0, r_1)$ previously introduced,

$$\theta_a(r) = \begin{cases} 1 & \text{if } r \leq a \\ 0 & \text{if } r > a \end{cases}$$

Then the function

$$\phi(|x|) = \xi(a) \theta_a(|x|)$$

is by construction such that

$$\phi(|x|) \leq V_a(|x|) \quad \text{for all } |x| \leq r_1$$

Let finally pose

$$\xi_1(|x|) = \xi(a) \chi_3\left(\frac{|x|}{a}\right)$$

Since $\chi_3(\frac{r}{a}) \leq \theta_a(r)$, we have that $\xi_1(r) \leq \phi(r) \leq \xi(r)$, for all $|x| \leq r_1$. Moreover

$$\tilde{\xi}_1(p) = a^d \xi(a) \tilde{\chi}_3(ap) \geq C^* \frac{a^d \xi(a)}{[(ap)^2 + 1]^d}$$

We can now bound the Fourier transform of $\Phi_2(|x|) = \xi_1(|x|) - \eta_3(|x|)$ as

$$\tilde{\Phi}_2(p) \geq \left[C^* a^d \xi(a) - C' \left[\frac{\pi^{\frac{d}{2}} (r_2 + r_1)^d}{\Gamma(\frac{d}{2} + 1)} w + H \right] \right] \frac{1}{[(ap)^2 + 1]^d} \quad (\text{A.12})$$

We may now choose our $a \in (0, r_1)$ such that

$$\xi(a) \geq \frac{C}{a^d} \quad (\text{A.13})$$

with

$$C = \frac{C'}{C^*} \left[\frac{\pi^{\frac{d}{2}} (r_2 + r_1)^d}{\Gamma(\frac{d}{2} + 1)} w + H \right]$$

which is always possible, since, due to the assumption (2.15), $\xi(|x|)|x|^d \rightarrow \infty$ as $|x| \rightarrow 0$. By inserting condition (A.13) into (A.12) we get that

$$\tilde{\Phi}_2(p) \geq 0$$

I.e. $\Phi_2(|x|)$ has a non-negative Fourier transform and so it is positive-definite. Hence, when a satisfies (A.13), $V_a(|x|) = \Psi_1(|x|) + \Psi_2(|x|)$, being the sum of a positive $\Psi_1(|x|)$ plus a positive-definite $\Psi_2(|x|)$ is, by the Ruelle criterium [26], a stable pair potential.

We can now conclude the proof of Proposition 1. We have proved above that $V_a(|x|)$ is stable. We note now that $V_a(|x|)$ is, by construction, absolutely summable (because $V_a(|x|)$ is bounded by $V(a)$ at short distances and moreover $V(|x|)$ is tempered). Hence we can write

$$V(|x|) = \Phi_1(|x|) + \Phi_2(|x|)$$

where $\Phi_1(|x|) = V(|x|) - V_a(|x|)$ non-negative and tempered (actually compact supported) and $\Phi_2(|x|) = V_a(|x|)$ stable and absolutely summable.

□

Acknowledgments

A. P. has been partially supported by the Brazilian agencies Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) and FAPEMIG (Fundação de Amparo à Pesquisa do Estado de Minas Gerais)-Programa Pesquisador Mineiro.

References

- [1] A. Abdesselam and V. Rivasseau (1995): *Tree forests and jungles: a botanical garden for cluster expansions in Constructive physics*, Proceedings, Palaiseau, France 1994, Lecture notes in physics n. 446.
- [2] N. Angelescu, G. Nenciu, V. Protopopescu (1971): *On stable potentials*. Commun. in Math. Phys. **22**, Issue 2, pp 162-165.
- [3] B. Addis and W. Schachinger (2010): *Morse potential energy minimization: Improved bounds for optimal configurations*, Comput. Optim. Appl. **47**, 129131.
- [4] D. Brydges and P. Federbush (1978): *A new form of the Mayer expansion in classical statistical mechanics*. J. Math Phys. **19**, 2064 (4 pages).
- [5] D. C. Brydges (1984): A short cluster in cluster expansions. In *Critical Phenomena, Random Systems, Gauge Theories*, Osterwalder, K. and Stora, R. (eds.), Elsevier, 129–83.
- [6] R. Fernández and A. Procacci (2007): *Cluster expansion for abstract polymer models. New bounds from an old approach*, Commun. Math Phys, **274**, 123–140.
- [7] R. Fernández; A. Procacci (2008): “Regions without complex zeros for chromatic polynomials on graphs with bounded degree”. *Comb. Prob. Comp.*, 17, 225–238.
- [8] R. Fernández, A. Procacci and B. Scoppola (2007): *The analyticity region of the hard sphere gas. Improved bounds*. Journal of Statistical Physics, **128**, 1139–1143.
- [9] M. E. Fisher and D. Ruelle (1966): *The Stability of Many-Particle Systems*, J. Math. Phys. **7**, 260–270.
- [10] G. Gallavotti (1999): *Statistical mechanics. A short treatise*, Springer Verlag.
- [11] J. Groeneveld (1962): *Two theorems on classical many-particle systems*. Phys. Lett., **3**, 50–51.
- [12] S. Jansen (2012): *Mayer and virial series at low temperature*, J. Stat. Phys. **147**, 678–706.
- [13] J. G. Kirkwood (1946): *The statistical mechanical theory of transport processes*, J. Chem. Phys., **14**, 180-201.
- [14] A. Lennard and S. Sherman (1970): *Stable Potentials, II*, Commun. Math. Phys., **17**, 91–97.
- [15] M. Locatelli and F. Schoen (2002): *Minimal interatomic distance in Morse clusters*, Journal of Global Optimization **22**, 175–190.
- [16] J. E. Mayer (1942): *Contribution to Statistical Mechanics*, J. Chem. Phys., **10**, 629–643.
- [17] J. E. Mayer and M. G. Mayer (1940): *Statistical Mechanics*, John Wiley & Sons, Inc. London: Chapman & Hall, Limited.
- [18] J. E. Mayer (1947): Integral equations between distribution functions of molecules, J. Chem. Phys., **15**, 187–201.

- [19] O. Penrose (1963): *Convergence of Fugacity Expansions for Fluids and Lattice Gases*, Journal of Mathematical Physics **4**, 1312 (9 pages).
- [20] O. Penrose (1963): *The Remainder in Mayer's Fugacity Series*, J. Math. Phys. **4**, 1488 (7 pages).
- [21] O. Penrose (1967): *Convergence of fugacity expansions for classical systems*. In *Statistical mechanics: foundations and applications*, A. Bak (ed.), Benjamin, New York.
- [22] S. Poghosyan and D. Ueltschi (2009): *Abstract cluster expansion with applications to statistical mechanical systems*, J. Math. Phys. **50**, no. 5, 053509, (17 pp).
- [23] A. Procacci (2007): *Abstract Polymer Models with General Pair Interactions*, arxiv.org/0707.0016 version 2 of 26 Nov. 2008.
- [24] A. Procacci (2009): *Erratum and Addendum: "Abstract Polymer Models with General Pair Interactions"*, J. Stat. Phys., **135**, 779–786.
- [25] A. Procacci, B. N. B. de Lima and B. Scoppola (1998): *A Remark on High Temperature Polymer Expansion for Lattice Systems with Infinite Range Pair Interactions*, Lett. Math. Phys., **45**, 303–322.
- [26] D. Ruelle (1969): *Statistical mechanics: Rigorous results*. W. A. Benjamin, Inc., New York-Amsterdam.
- [27] D. Ruelle (1963): *Correlation functions of classical gases*, Ann. Phys., **5**, 109–120.
- [28] D. Ruelle (1963): *Cluster Property of the Correlation Functions of Classical Gases*, Rev. Mod. Phys., **36**, 580–584.
- [29] S. Tate (2013): *Virial Expansion Bounds*, J. Stat. Phys. **153**, 325–338.